The role of Berry phase in the spectrum of order parameter dynamics: a new perspective on Haldane's conjecture on antiferromagnetic spin chains

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We formulate the dynamics of local order parameters by extending the recently developed adiabatic spinwave theory involving the Berry curvature, and derive a formula showing explicitly the role of the Berry phase in determining the spectral form of the low-lying collective modes. For antiferromagnetic spin chains, the Berry phase becomes a topological invariant known as the Chern number. Our theory predicts the existence of the Haldane gap for a topologically trivial ground state, and a linear dispersion of low-lying excitations for a non-trivial ground state.

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Ever since Landau's formulation of continuous phase transition, the study of order parameter and its associated dynamics has occupied a central part of modern physics. Dynamics of the order parameter gives rise to collective excitations known as Goldstone modes, with important consequences on thermal, mechanical, electrical or magnetic properties of physical systems. Also, the absence of symmetry breaking in lower dimensional systems at finite temperatures can be understood as a result of thermal fluctuations of the low-lying modes of the order parameter dynamics. For many one-dimensional systems, there exist well-defined collective modes, such as the 'spinwaves' in the antiferromagnetic Heisenberg spin chain [1], even though the ground state is disordered. It is very attempting to regard these collective modes also as that of the order parameter dynamics while the destruction of the long range ordering in the ground state is attributed to their quantum fluctuations [2].

In this Letter, we formulate a theory of order parameter dynamics based on the local ordering in the system alone. We follow the approach of Ref. [3] for symmetry breaking magnetic systems to derive the equations of motion and a formula for the collective excitation spectrum:

$$\hbar\omega = \frac{\Delta E}{B}, \tag{1}$$

where ΔE is the energy increase from the ground state for a frozen configuration of the order parameter and B is the Berry phase of the many-body wave function during a cycle of the collective motion. We apply our theory to the systems of antiferromagnetic spin chains, showing that the presence or absence of a Haldane gap [4] is directly tied to a topological charge in the ground state.

Haldane conjectured that the excitations of an antiferromagnetic Heisenberg chain have a gap for spins of integer S and are gapless for spins of half-integer values [4]. This was based on a mapping to a nonlinear sigma-model in the large S limit, where a topological action term is present for half-integer spins but not for integer spins. Without the topological term, the nonlinear sigma-model was known to be gapped, but a rather elaborate renormalization group analysis was needed to show that the presence of the topological term can render the excitations gapless [5]. Haldane's conjecture seems to be correct also for small spins, because it conforms with the exact solutions for the extreme cases of $S = 1/2$ [1] and $S = 1$ [6] and with numerical results. The success of Haldane's conjecture is highly celebrated in the theoretical physics community, because it gives a prime example that topology can play such a decisive role in measurable effects.

Here we present a direct mechanism showing how topology works its way to determine the spectral form of the excitations. For the antiferromagnetic chains, we will show that the Berry phase for a mode of wave number k can be written for small k as

$$B \propto \frac{kL}{2\pi}Q + O(k^2), \tag{2}$$

where L is the length of the chain and Q is the topological charge defined as the Chern number of the wave function mapped to the order parameter configuration in the excitation mode. On the other hand, the energy increase in a frozen configuration of the order parameter should have the form

$$\Delta E \propto Lk^2. \tag{3}$$

Therefore, depending on the presence or absence of this topological charge Q, the excitation spectrum is linearly dispersed for small k or becomes gapped:

$$\hbar\omega \propto \begin{cases} k, & \text{if } Q \neq 0; \\ \Delta, & \text{if } Q = 0, \end{cases} \tag{4}$$

where Δ is a constant. In many one dimensional antiferromagnetic models of integer spin, such as the AKLT model for $S = 1$ [6] and its SU(N) generalization [7], the exactly soluble ground states are topologically trivial ($Q = 0$). On the other hand, several spin half-integer models have been constructed with topologically non-trivial ground states, e.g., the resonating-valence-bond

ground state with a twofold degeneracy in the spin-Pereils order [7]. The Lieb-Schultz-Mattis theorem for spin-half and its generalization to arbitrary half-integer spins [8] also indicated this non-triviality. In lights of these facts and the general arguments given in Ref. [9], we can thus conclude that our spectral formula is really consistent with Haldane's conjecture [4].

The standard procedure of introducing the order parameter is to apply a weak external field to force the system to order in a particular way, corresponding to some non-zero expectation value of the operator in conjugation to the field $\varphi_x^j = \langle \hat{O}_x^j \rangle$, where x denotes the position and j labels the internal components. If the ordering persists after the field is turned-off, we say that there is a spontaneous symmetry breaking, and the nonzero expectation value is called the order parameter. Standard examples of order parameter include the magnetization field in magnetic materials, the condensate wave function for superfluids [10], the Ginzburg-Landau order parameters in superconductivity [11] and many other condensed matter systems [12]. To facilitate the discussion of its dynamics, we generalize the notion by defining the order parameter in any state simply as the expectation value of $\hat{O}_x^j$ in that state. In this way, we can also talk about the order parameter even for systems without long range order.

As long as there is a strong local ordering, the low-lying excitations should be dominated by the order parameter dynamics in the following sense. Consider the set of constrained ground states defined as the union of the lowest energy state for each configuration of the order parameter. If an initial state prepared from this set will evolve entirely within this set, then we have a closed dynamics of the order parameter because such states are labeled uniquely by the order parameter configuration. We assume this is the case, which can be justified at least for those long wavelength deviations of the ground state configuration. We can then apply the time dependent variational principle along the line of Refs. [3,13] to derive the equations of motion of the order parameter dynamics

$$\sum_{j',x'} \hbar \Omega^{jj'}_{xx'} \dot{\varphi}^{j'}_{x'} = \frac{\partial E}{\partial \varphi^j_x}, \tag{5}$$

which involve the energy $E = \langle \psi | H | \psi \rangle$ of the constrained ground state and the Berry curvature

$$\Omega^{jj'}_{xx'} = \frac{\partial}{\partial \varphi^j_x} \langle \psi | \frac{i\partial}{\partial \varphi^{j'}_{x'}} | \psi \rangle - \frac{\partial}{\partial \varphi^{j'}_{x'}} \langle \psi | \frac{i\partial}{\partial \varphi^j_x} | \psi \rangle. \tag{6}$$

The spectral formula (1) can be derived directly from the equations of motion. In Ref. [13], the formula was obtained for the case of spinwave by linearizing the equations of motion around the ground state for ferro-, ferri- and antiferromagets. There it was also shown that this Berry phase is actually given by the reduction of the total magnetization from the ground state due to the spinwave, thus proving and generalizing an earlier result from Ref. [3] for the spinwave spectrum. This formula has now served the basis for a number of successful first principle calculations for ferromagnetic crystals [14], and similar work on other types of magnetic materials are expected in the near future. Exactly the same derivation of the spectral formula can be applied for the order parameter dynamics of any system with a symmetry breaking ground state. The same reasoning should also give the Berry phase in terms of the deviation from the ground state expectation value of the generator of the collective motion.

For a system with no spontaneous breaking of symmetry, such as the antiferromagnetic chain, the spectral formula (1) still stands as shown by the following arguments. We multiply both side of (5) by $dt\, \delta_E \varphi^j_x$ and sum over x and j, i.e.

$$\sum_{a,a'} \hbar \Omega_{aa'} \frac{\partial \varphi^{a'}}{\partial t} dt\, \delta_E \varphi^a = \sum_a \frac{\partial E}{\partial \varphi^a}\, dt\, \delta_E \varphi^a, \tag{7}$$

where the two labels have been condensed into one for simplicity ($\varphi^a \equiv \varphi^j_x$), and $\delta_E \varphi^a$ is the variation in a direction perpendicular to the constant energy trajectory of the order parameter. We then integrate (7) over the two-dimensional domain $\mathcal{D}_\varphi$ consisting of a one parameter family of trajectories ranging from the fixed point in the absolute ground state to a trajectory $\mathcal{C}_\varphi$ of finite amplitude of the collective motion. In the harmonic regime, where the collective modes may be defined, we expect that the time period T to be a constant, so that the integration yields

$$\hbar \int_{\mathcal{D}_\varphi} \sum_{aa'} \delta_t \varphi^a \delta_E \varphi^{a'} \Omega_{aa'} = T \Delta E, \tag{8}$$

where $\Delta E = E - E_0$ is the energy increase from the ground state, and $\delta_t \varphi^a$ denotes the variation of the order parameter along the trajectory (i.e., $\delta_t = dt\partial/\partial t$). Because the time period T relates to the frequency ω of the collective mode by $T = \frac{2\pi}{\omega}$, we arrive at the formula (1) with the Berry phase given by

$$\begin{aligned} B &= \frac{1}{2\pi} \int_{\mathcal{D}_\varphi} \sum_{aa'} \delta_t \varphi^a \delta_E \varphi^{a'} \Omega_{aa'} \\ &= \frac{1}{2\pi} \oint_{\mathcal{C}_\varphi} \sum_a \delta_t \varphi^a \langle \psi | \frac{i\partial}{\partial \varphi^a} | \psi \rangle. \end{aligned} \tag{9}$$

where the second equality results from the Stokes theorem.

To appreciate how the Berry phase determines the spectral form of the low-lying collective mode, we expand it in powers of the wave number k

$$B = B_0 + B_1 k + B_2 k^2 + ... \tag{10}$$

For ferro- and ferrimagnets, we have $B_0 \neq 0$ because the total magnetization reduction due to a spinwave is nonzero even in the limit of zero k. This yields a quadratic dispersion for the spectrum at small k in light of Eq.(3). For lattices with antiferromagnetic ordering, we have $B_0 = 0$ due to sublattice symmetry [7], while $B_1 \neq 0$ [15] from a careful analysis of magnetization reduction in the presence of a spinwave of small but nonzero k. This reproduces the standard result that antiferromagnetic spinwaves have a linear dispersion at small k.

For antiferromagnetic spin chains, where the spin rotation symmetry cannot be spontaneously broken according to Coleman's theorem, the results drawing from the total spin reduction may not be applicable. Fortunately, we have two observations that help to establish the topological interpretation of the Berry phase shown in (2). First, the total Berry phase due to a cyclic motion in the order parameter configuration space can be expressed as a sum of the Berry phases due to the cyclic motion of local order parameter at each site. In other words, we may write the Berry phase (9) in the form

$$B = \sum_x \frac{1}{2\pi} \oint_{C_x} \delta_t \vec{\varphi}_x \cdot \langle\psi| \frac{i\partial}{\partial \vec{\varphi}_x} |\psi\rangle, \tag{11}$$

where C_x denotes the path of the local spin moment $\vec{\varphi}_x$ as the projection of the configurational path $\mathcal{C}_\varphi$ on site x. For each term in the sum, the constrained ground state $|\psi\rangle$ is evaluated with the spin moments on all sites except x set to their true ground state value, i.e., zero. This observation may fail for itinerant spin systems such as the $t-J$ model, because the Berry curvature is known to have inter-site terms which prevent the resolution of the Berry phase into contributions from each site. However, we expect the observation to be true for localized spin systems such as the Heisenberg model.

A direct consequence of the above observation is that the total Berry phase (11) can be written as the number of the space periods, $n = \frac{kL}{2\pi}$, times the Berry phase in one period, [16]

$$B = \frac{k}{2\pi} L B_{\rm p}, \tag{12}$$

where L is the size of the chain and B_p is defined by (11) but with the sum over x confined in one space period $(0, \lambda)$. Our second observation then shows that B_p is proportional to a topological charge. We note that because of the local antiferromagnetic ordering, the directions of spin moments on neighboring sites tend to be opposite to each other, so is the sense of chirality of their motion. Therefore, the contributions to the Berry phase from neighboring sites almost cancel each other for long wavelength collective modes. It will thus be convenient to introduce the staggered order parameter $\vec{m}_x = (-1)^x \vec{\varphi}_x$, so that the Berry phase per period becomes

$$B_p = \frac{1}{2\pi} \sum_{x\in(0,\lambda)} (-1)^x \oint_{C'_x} \delta_t \vec{m}_x \cdot \langle\psi| \frac{i\partial}{\partial \vec{m}_x} |\psi\rangle, \tag{13}$$

where C'_x denotes the orbit of $\vec{m}_x$. For small k, we may take the continuum limit by replacing the difference by a differential,

$$B_p = \frac{1}{2\pi} \sum_{x\in(0,\lambda)} \oint_{C'_x} \delta_t \vec{m}_x \cdot \sum_j \delta_x m_x^j \left[\frac{\partial}{\partial m_x^j} \langle\psi| \frac{i\partial}{\partial \vec{m}_x} |\psi\rangle - \frac{\partial}{\partial \vec{m}_x} \langle\psi| \frac{i\partial}{\partial m_x^j} |\psi\rangle \right], \tag{14}$$

where δ_x stands for $dx \frac{\partial}{\partial x}$ and the second term is an added zero term. Due to the spatial periodicity, the sum over x corresponds to a closed loop integral, so that (14) becomes an integral over the closed space-time torus T^2

$$B_p \equiv Q = \frac{1}{2\pi} \oint_{T^2} \sum_{j,j'} \delta_x m_x^j \delta_t m_x^{j'} \Omega_{jj'}(\vec{m}_x), \tag{15}$$

with the curvature

$$\Omega_{jj'}(\vec{m}) = \frac{\partial}{\partial m^j} \langle\psi| \frac{i\partial}{\partial m^{j'}} |\psi\rangle - \frac{\partial}{\partial m^{j'}} \langle\psi| \frac{i\partial}{\partial m^j} |\psi\rangle. \tag{16}$$

Thus, the Berry phase per spatial period of a collective excitation in an antiferromagnetic spin chain is in fact a topological invariant, the first Chern class for the mapping of the constrained ground state to the space-time structure of the local order parameter. This reduces to the standard semiclassical result of

$$Q = \frac{1}{2\pi} \oint_{T^2} \delta_x \vec{m} \times \delta_t \vec{m} \cdot \vec{m}/|\vec{m}|^2, \tag{17}$$

if we take $\Omega_{jj'} = \sum_l \epsilon_{jj'l} m^l/|\vec{m}|^2$. Our expression (15) is a generic result and model-independent. It has been expected that the topology of the ground states of spin chains is trivial for integer S but non-trivial for half-integer S [9]. For an $S = 1$ chain, the authors of Ref. [6] provided an exact valence-bond-solid ground state which is topologically trivial [6]. Read and Sachdev discussed the SU(N) antiferromagnetic chains in the large N limit [7]. By using a trial ground state wave function, they showed that there is a spin-Peierls order parameter proportional to the topological charge of the ground state. They explicitly gave the dependence of the ground state energies on the topology of the state. They concluded that the valence-bond-solid ground state of the integer spin chains is topologically trivial and not degenerate with a vanishing spin-Pereils order parameter; The resonating-valence-bond ground state for the half-integer chains, on the other hand, is topologically nontrivial and degenerate due to the different spin-Pereils order parameters. We can also see the topological property of the chains in the twist introduced in [8], which, in some sense, gave a finite S version of the topological term in the nonlinear sigma model [17].

Our spectral formula eq.(1) can also serve the basis for numerical calculation of the excitation spectrum. A quantitative comparison of the numerical result with known theoretical and experimental results should constitute a stringent test of our theory. For example, in the spin-1/2 antiferromagnetic chain, the spinwave speed is $\pi/2$ times larger than the semiclassical result [1], and it would be interesting to see if the numerical calculation based on our formula will give the correct result.

In conclusion, we have formulated a theory of local order parameter dynamics and derived a formula for the spectral form of collective excitations in terms of the Berry phase. For antiferromagnetic spin chains, we have shown in a model-independent manner that the presence or absence of a gap is directly tied to the topological structure of the constrained ground state. For all known exact or model solutions of the spin chains, our result is consistent with Haldane's conjecture. We also recognize that the topological consideration may not be valid for itinerant spin systems because of the non-vanishing inter-site Berry curvature.

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